Bis(phenylsulfonyl)methane

Other names: Benzene, 1,1'-[methylenebis(sulfonyl)]bis-
[methylenebis(sulphonyl)]bisbenzene
Inchi: InChI=1S/C13H12O4S2/c14-18(15,12-7-3-1-4-8-12)11-19(16,17)13-9-5-2-6-10-13/h1-10
InchiKey: QCHNSJNRFSOCLJ-UHFFFAOYSA-N
Formula: C13H12O4S2
SMILES: O=S(=O)(CS(=O)(=O)c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 296.36
CAS: 3406-02-8

Physical Properties

Property code	Value	Unit	Source
gf	-653.68	kJ/mol	Joback Method
hf	-745.29	kJ/mol	Joback Method
hfus	40.26	kJ/mol	Joback Method
hvap	86.35	kJ/mol	Joback Method
log10ws	-2.58		Crippen Method
logp	1.892		Crippen Method
mcvol	202.690	ml/mol	McGowan Method
pc	4480.21	kPa	Joback Method
tb	645.76	K	Joback Method
tc	869.33	K	Joback Method
tf	366.23	K	Joback Method
vc	0.799	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	493.24	J/mol×K	645.76	Joback Method
cpg	508.95	J/mol×K	683.02	Joback Method
cpg	523.35	J/mol×K	720.28	Joback Method
cpg	536.44	J/mol×K	757.55	Joback Method
cpg	548.26	J/mol×K	794.81	Joback Method
cpg	558.83	J/mol×K	832.07	Joback Method
cpg	568.16	J/mol×K	869.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3406028&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume